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Request for Information from entities interested in commercializing Laboratory-developed homogeneous catalyst technology Title:

Author(s): Intrator, Miranda Huang

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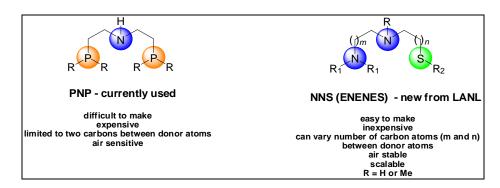
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# Request for Information from entities interested in commercializing Laboratory-developed homogeneous catalyst technology

Los Alamos National Security, LLC (LANS) is the manager and operator of Los Alamos National Laboratory (Los Alamos) for the U.S. Department of Energy National Nuclear Security Administration under contract DE-AC52-06NA25396. Los Alamos is a mission-centric Federally Funded Research and Development Center focused on solving critical national security challenges through science and engineering for both government and private customers. LANS is opening this formal Request for Information (RFI) to gauge interest in engaging as an industry partner to LANS for collaboration in advancing the bio-assessment platform described below. Please see last section for details on submitting a Letter of Interest.



### A VERSATILE LIGAND AND METAL COMPLEX TOOLBOX

Many industrial catalysts used for homogeneous hydrogenation and dehydrogenation of unsaturated substrates are derived from metal complexes that include (air-sensitive) ligands that are often expensive and difficult to synthesize. In particular, catalysts used for many hydrogenations are based on phosphorus containing ligands (in particular PNP pincer systems). These ligands are often difficult to make, are costly, are constrained to having two carbon atoms in the ligand backbone and are susceptible to oxidation at phosphorus, making their use somewhat complicated. Los Alamos researchers have recently developed a new and novel set of ligands that are based on a NNS (ENENES) skeleton (i.e. no phosphorus donors, just nitrogen and sulfur). Advantages of these ligands include:

- Ease of synthesis from commercially available, inexpensive starting materials at the multi-gram scale;
- Scalability of synthesis (multi-gram quantities are easily accessible in one loading);
- Ability to readily change the number of carbon atoms in ligand backbone (unlike PNP systems);
- Tunability of electronics and sterics (e.g. facile addition of various substituents at N and S centers);
- Chirality;
- Air stability;
- Demonstrated good activity in carbonyl group hydrogenations;
- Potential activity in numerous other catalytic reaction (see below).



#### LIGANDS AND COMPLEXES FOR HOMOGENEOUS CATALYSIS

Los Alamos scientists have prepared new ligands from inexpensive starting materials, and new metal complexes with these ligands, investigating their activity and selectivity towards the hydrogenation of carbonyl containing species (e.g. esters). Several structurally unprecedented catalysts were synthesized, and hydrogenation of esters and ketones has been demonstrated with high selectivity. This technology represents a new alternative to PNP-based systems that may have the potential for efficacy in numerous catalytic reactions, including but not limited to:

- Asymmetric catalysis
- Hydrogenating unsaturated substrates, e.g.:
  - Alkenes
  - Alkynes
  - Carbonic & carboxylic acid derivatives
  - CO<sub>2</sub>
  - Esters
  - Fluorinated esters
  - Heterocycles
  - Imines
  - Ketones
  - Formates
  - Cyclic carbonates

- Catalytic hydrolysis or dehydrogenation of ammonia or amine boranes
- Various acceptorless dehydrogenations
- Various dehydrations
- Polymerizing alkenes
- Transfer hydrogenation of organic formates and cyclic carbonates
- Domino-synthesis of indoles
- Stereospecific polymerization of 1,3-butadiene
- Ethylene tetra- and trimerisation
- CO<sub>2</sub> transfer hydrogenation of ketones
- Other types of catalysis

# POTENTIAL AREAS FOR PARNTERSHIP

- Design of scale-up synthetic chemistry to produce catalysts and/or ligands for large-scale distribution.
- Test & evaluation of catalysts and/or ligands for applications in the Pharmaceutical, Petrochemical & renewable energy, Agrochemical, Consumer products, Fine chemicals, Polymers, Flavors & fragrances, Advanced materials, Bioderived materials, Biologics, or other industries.
- Vending of the catalysts and/or ligands to third parties.

Please note this list is non-exhaustive. LANS welcomes Letters of Interest from any suitable party, and is not necessarily limited to one partner per area of interest.

## LANS INTELLECTUAL PROPERTY

- Polydentate ligands and their complexes for molecular catalysis (LANS Ref. No. S 133,200; PCT App. No. PCT/US2015/034793)
- Catalytic hydrogenation using complexes of base metals with tridentate ligands (LANS Ref. No. S 129,408; U.S.



Pat. App. No. 13/587,717)

Please note that the U.S. Government retains a worldwide, royalty-free, non-exclusive right to practice any LANS-owned patents and/or copyrighted software. Accordingly, any entity will have open access to LANS patents and copyrights in performance of a Government contract.

# **SUBMITTING A LETTER OF INTEREST**

This RFI is made without prejudice to any form of collaborative arrangement, alliance, or number of entities. *Ability and willingness to ensure compliance with U.S. Export Control law is a requirement*. Please submit a written response on how your organization envisions utilizing this technology in partnership with Los Alamos. This may include a business or product plan, a business model, information regarding your company, or any other type of relevant information. Please properly mark any information that is considered proprietary or business-sensitive. LANS will supply a Nondisclosure Agreement to any U.S. company or person requiring it. Those companies interested in pursuing this opportunity should direct a Letter of Interest, as well as any comments or questions, to <a href="mailto:catalysis@lanl.gov">catalysis@lanl.gov</a> before 11:59 MST on <a href="mailto:CDATE">CDATE</a>.

